

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
 Data File : BM033319.D
 Acq On : 06 Dec 2021 19:12
 Operator : CG/JU
 Sample : M4918-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-40

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM033319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.655	49	54	62	rVB	288583	377061	4.64%	0.883%
2	4.355	166	173	179	rBV2	141540	234631	2.89%	0.550%
3	4.419	179	184	186	rVV	117207	157954	1.94%	0.370%
4	4.449	186	189	199	rVB	144223	208846	2.57%	0.489%
5	5.507	364	369	380	rVB	1112929	1696169	20.86%	3.973%
6	6.196	475	486	495	rVB9	29151	87319	1.07%	0.205%
7	7.101	633	640	651	rBV	650078	1115786	13.72%	2.613%
8	7.343	672	681	688	rVB4	81827	190063	2.34%	0.445%
9	7.925	773	780	787	rBV	470244	756494	9.30%	1.772%
10	8.019	791	796	799	rVV3	51622	87500	1.08%	0.205%
11	8.090	800	808	816	rVB	152345	415940	5.12%	0.974%
12	8.231	816	832	838	rBV	461610	1343809	16.53%	3.147%
13	8.931	935	951	954	rBV2	381693	1099972	13.53%	2.576%
14	9.037	962	969	972	rBV	720284	1479945	18.20%	3.466%
15	9.084	972	977	985	rVB	1865860	3682483	45.29%	8.625%
16	9.725	1076	1086	1097	rVB	188422	424303	5.22%	0.994%
17	10.231	1164	1172	1177	rBV2	44511	100788	1.24%	0.236%
18	10.719	1248	1255	1269	rBV	611724	1109367	13.64%	2.598%
19	12.589	1566	1573	1576	rBV2	133403	249735	3.07%	0.585%
20	12.701	1587	1592	1605	rVB5	170138	430750	5.30%	1.009%
21	12.966	1632	1637	1642	rVB	75863	111528	1.37%	0.261%
22	13.172	1662	1672	1678	rBV	4028726	5946563	73.13%	13.928%
23	13.307	1687	1695	1702	rBV	74386	146088	1.80%	0.342%
24	13.560	1733	1738	1752	rBV	167545	328572	4.04%	0.770%
25	13.672	1753	1757	1764	rVB2	62862	98889	1.22%	0.232%
26	13.772	1765	1774	1779	rBV3	125647	288087	3.54%	0.675%
27	14.036	1814	1819	1824	rBV	70218	116647	1.43%	0.273%
28	14.177	1836	1843	1849	rVB2	133633	229024	2.82%	0.536%
29	14.360	1867	1874	1880	rBV	136214	232867	2.86%	0.545%
30	14.548	1896	1906	1913	rBV	893559	1421460	17.48%	3.329%
31	16.036	2152	2159	2171	rBV	2991880	4611406	56.71%	10.801%
32	17.283	2366	2371	2378	rBV	1071896	1638837	20.15%	3.838%
33	18.165	2518	2521	2531	rBV2	86317	149183	1.83%	0.349%
34	19.895	2809	2815	2822	rBV	6556191	8131622	100.00%	19.046%
35	21.142	3024	3027	3036	rBV3	138584	183555	2.26%	0.430%
36	21.442	3074	3078	3085	rBV	1427258	1896003	23.32%	4.441%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.777	3469	3475	3484	rVB2	938057	1915632	23.56%	4.487%
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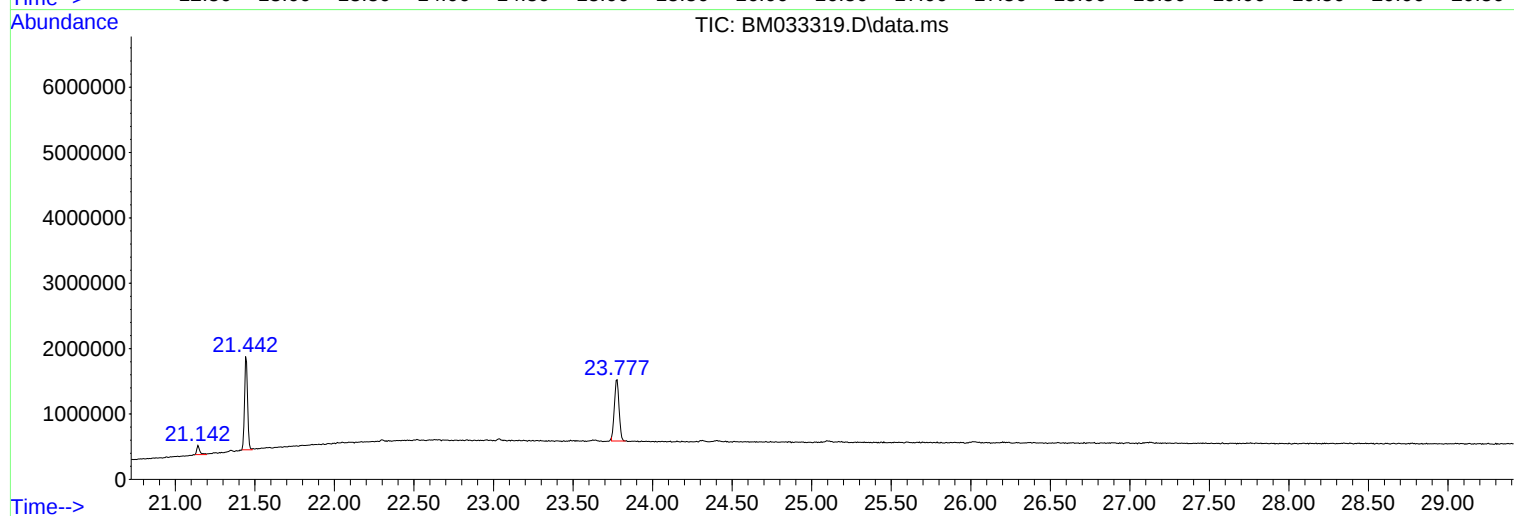
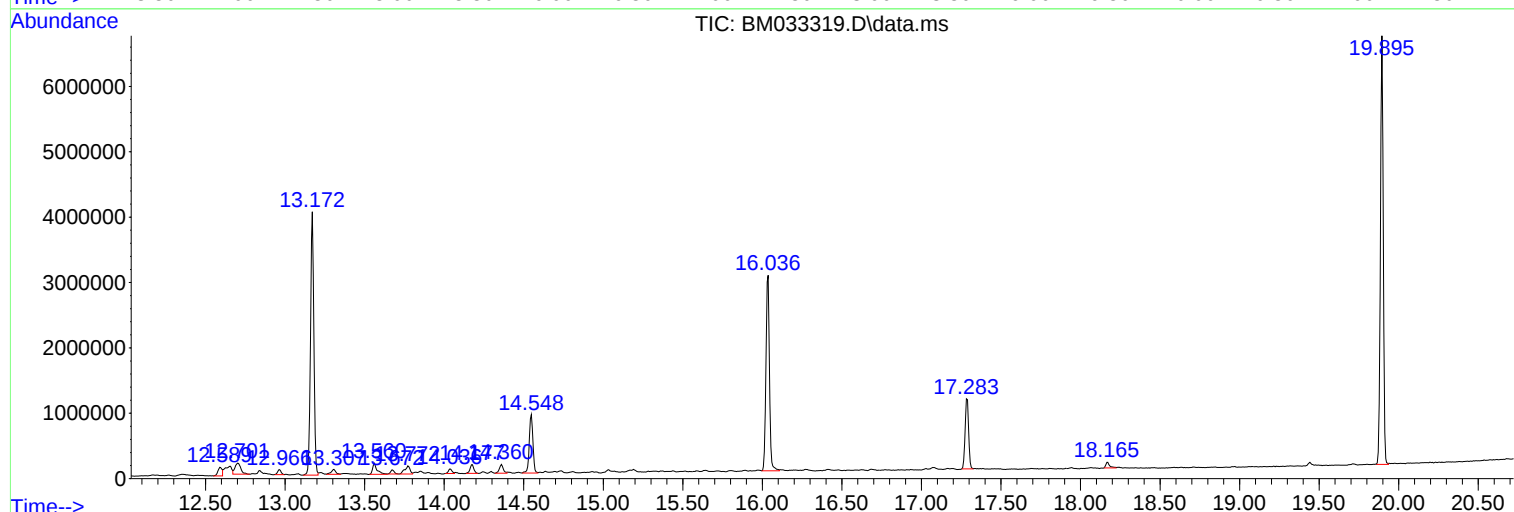
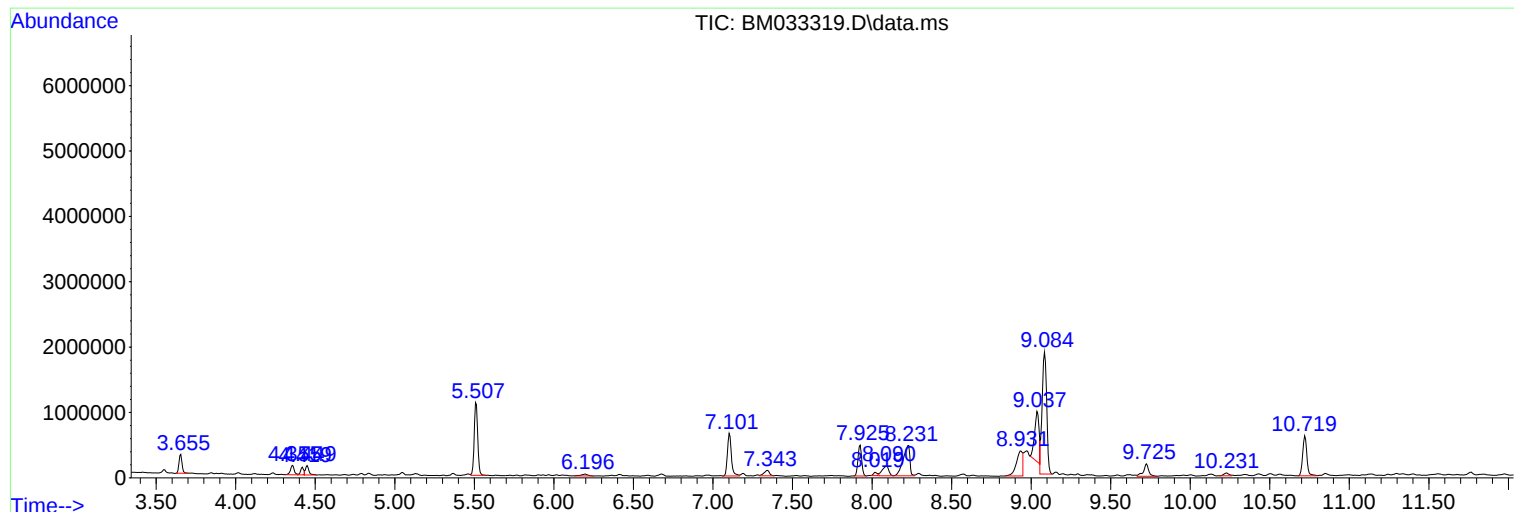
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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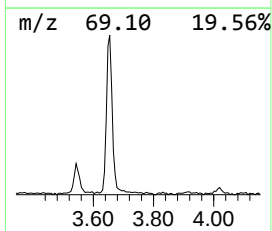
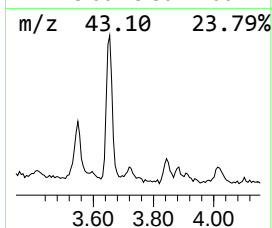
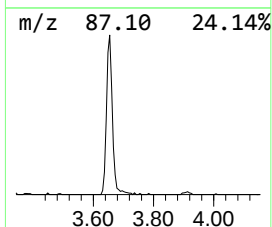
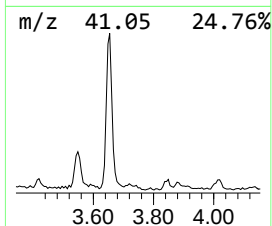
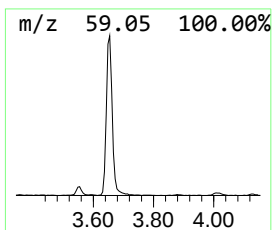
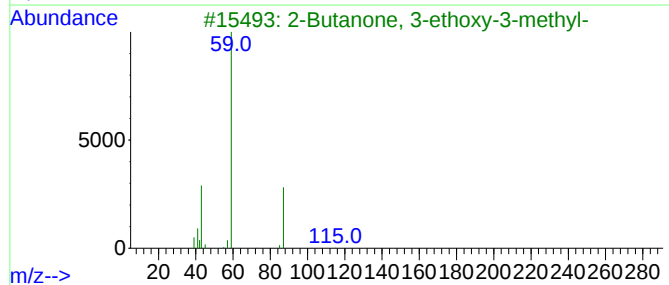
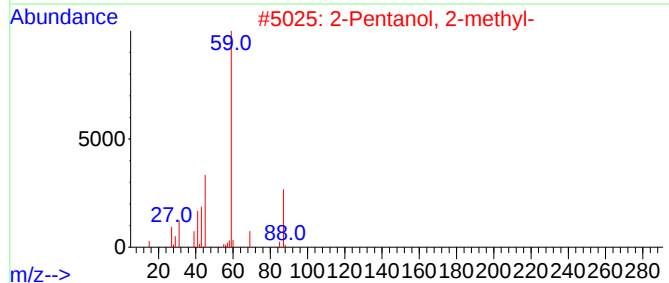
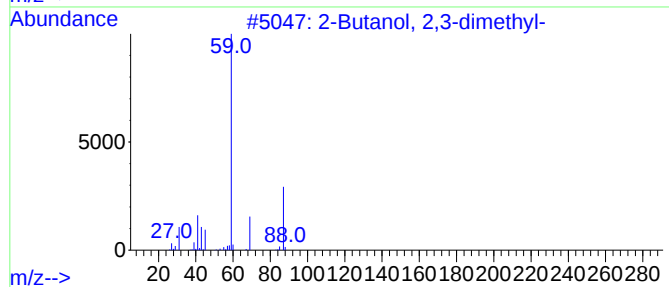
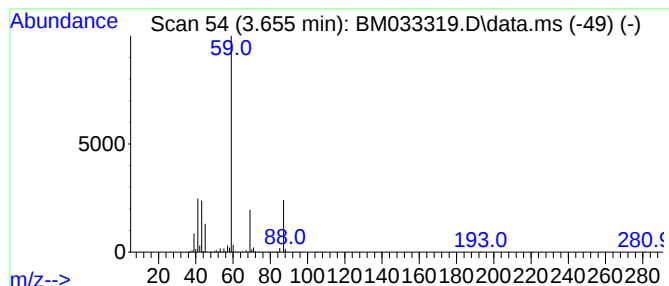
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.655	9.97 ng	377061	1,4-Dichlorobenzene-d4	7.925

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	74
3		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	50
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
5		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40



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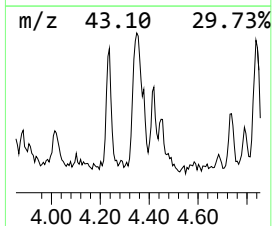
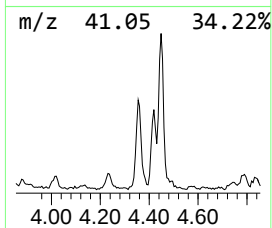
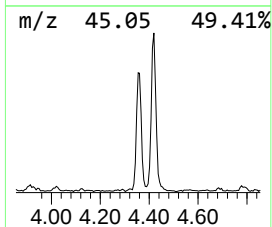
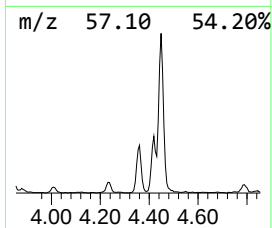
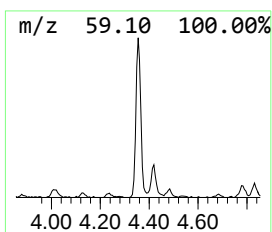
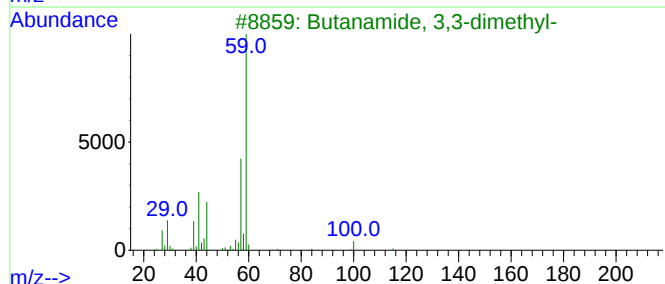
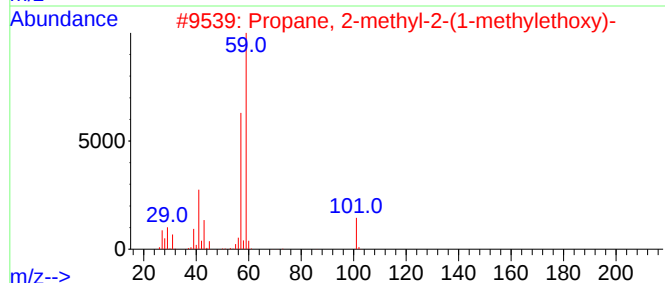
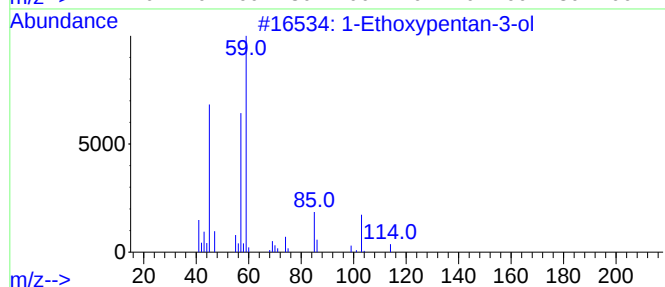
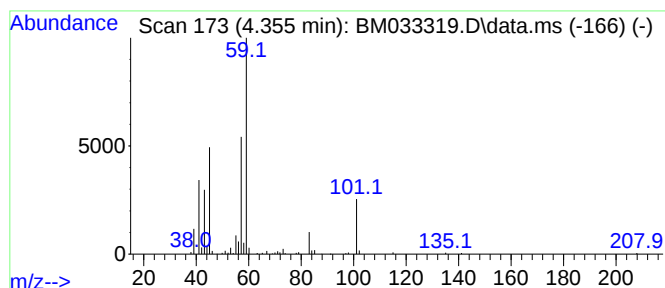
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Peak Number 2 1-Ethoxypentan-3-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.355	6.20 ng	234631	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethoxypentan-3-ol	132	C7H16O2	100910-92-7	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	43
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	42
5			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42



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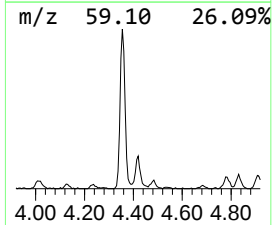
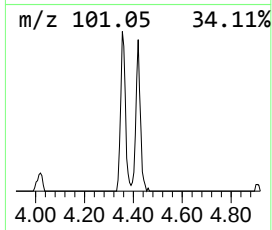
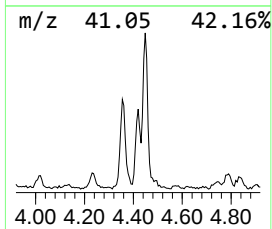
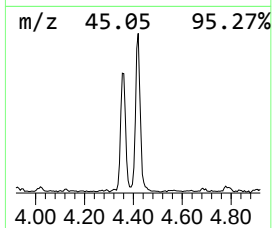
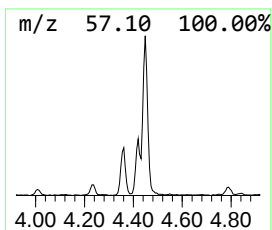
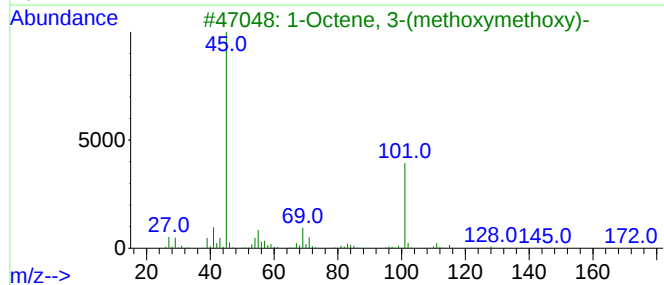
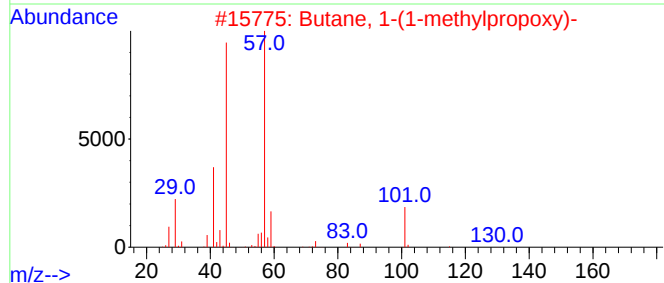
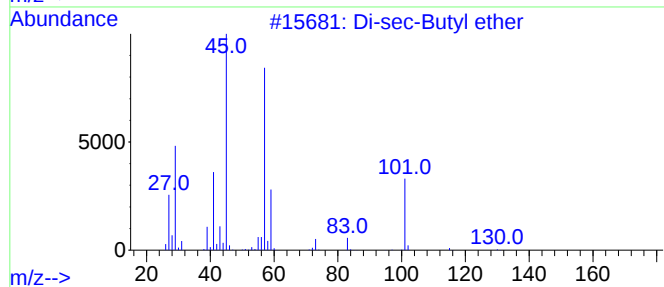
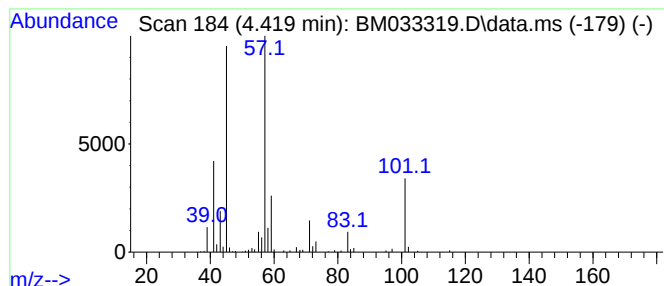
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Di-sec-Butyl ether Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.419	4.18 ng	157954	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	78
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
3			1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	47
4			3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	42
5			Hexane, 1,6-dimethoxy-	146	C8H18O2	013179-98-1	37



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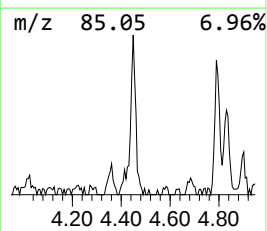
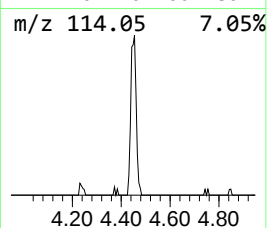
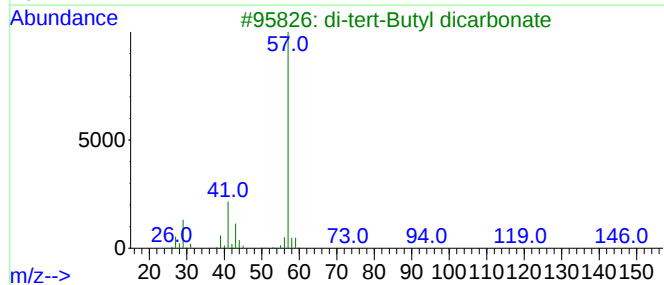
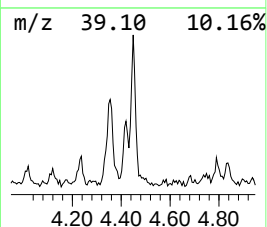
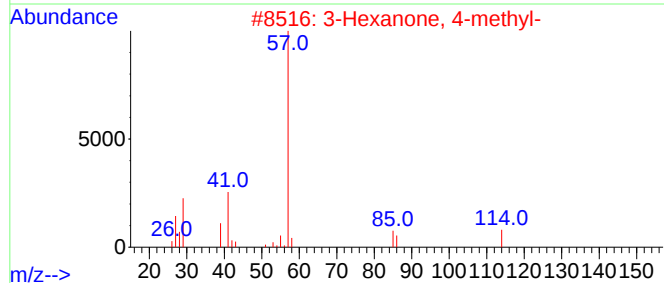
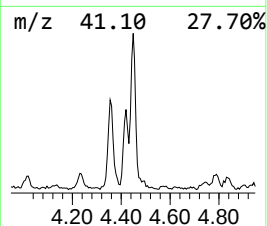
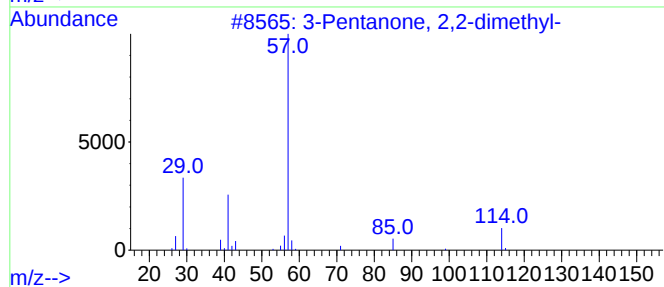
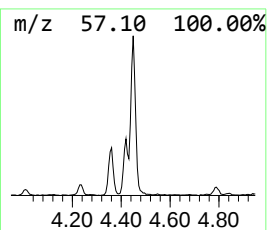
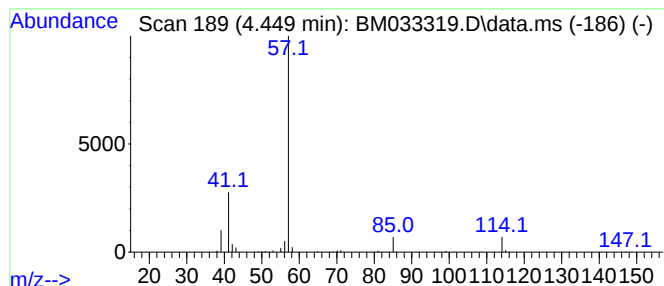
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 3-Pentanone, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.449	5.52 ng	208846	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	64
2			3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	50
3			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	28
4			3,4-Hexanedione	114	C6H10O2	004437-51-8	9
5			3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	9



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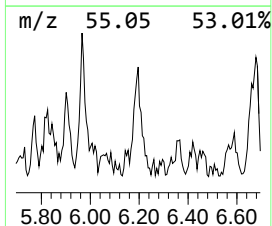
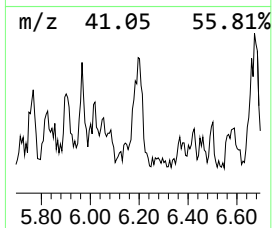
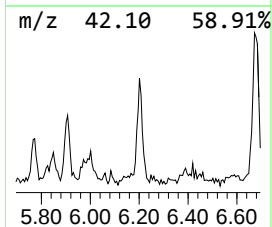
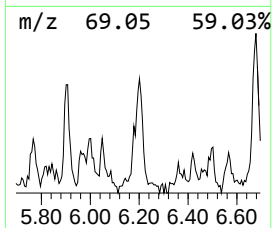
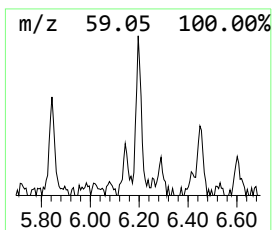
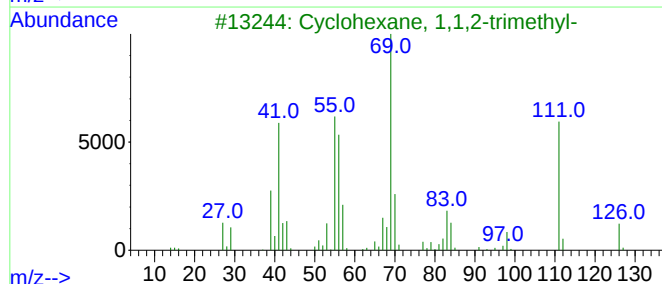
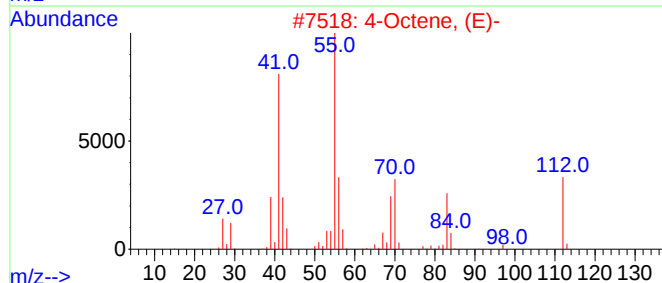
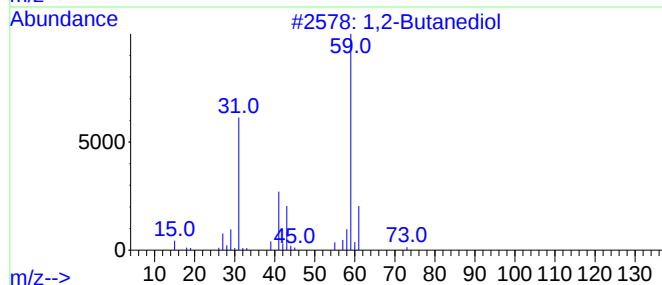
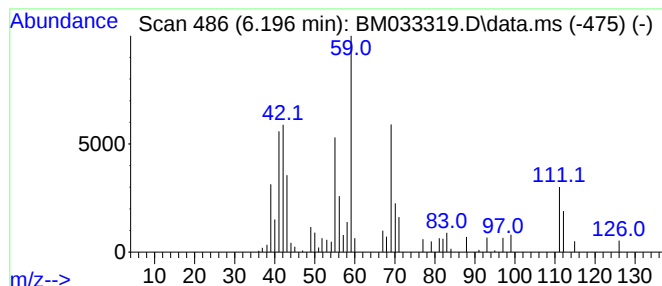
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown6.196 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.196	2.31 ng	87319	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Butanediol	90	C4H10O2	000584-03-2	27
2			4-Octene, (E)-	112	C8H16	014850-23-8	18
3			Cyclohexane, 1,1,2-trimethyl-	126	C9H18	007094-26-0	18
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	18
5			3-Octene, (E)-	112	C8H16	014919-01-8	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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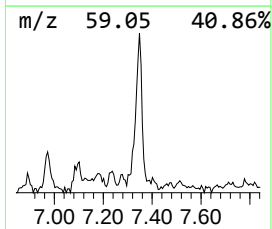
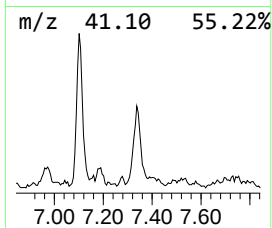
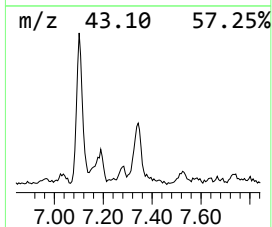
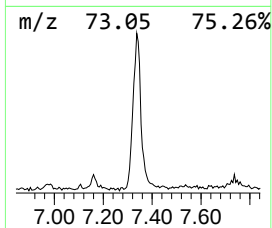
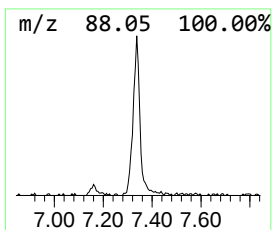
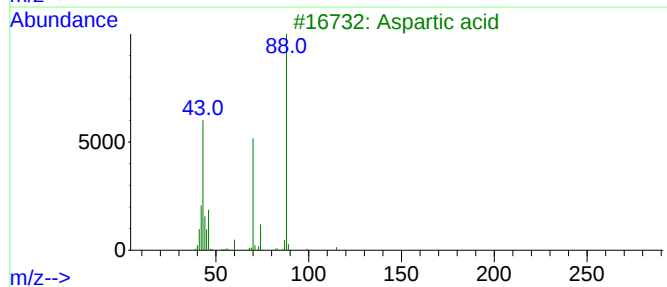
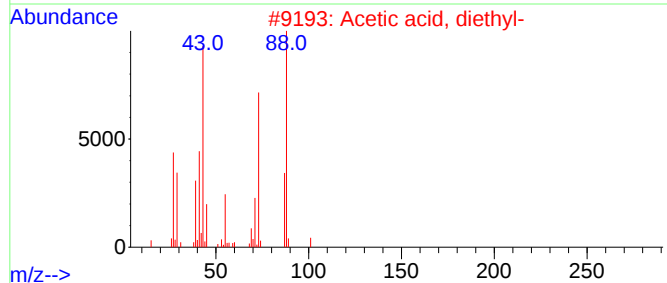
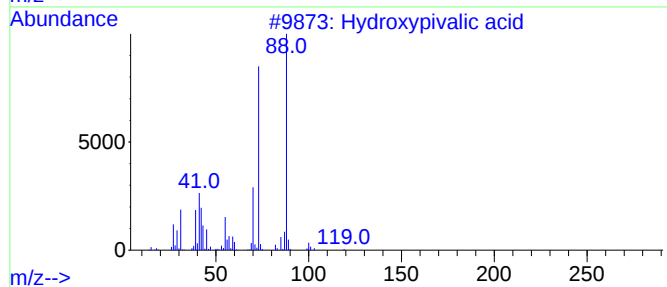
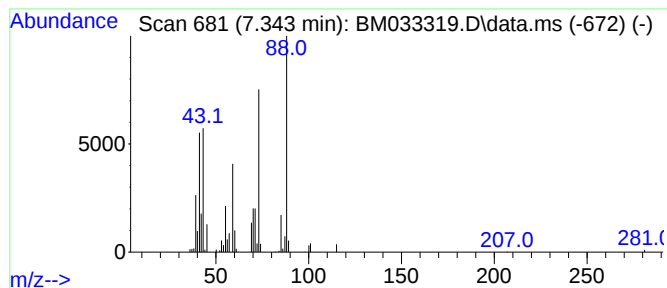
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hydroxypivalic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.343	5.02 ng	190063	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydroxypivalic acid	118	C5H10O3	004835-90-9	50
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	40
3			Aspartic acid	133	C4H7NO4	000056-84-8	38
4			Hexanoic acid, ethyl ester	144	C8H16O2	000123-66-0	38
5			Urea, ethyl-	88	C3H8N2O	000625-52-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
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Sample : M4918-06
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Instrument :
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ClientSampleId :
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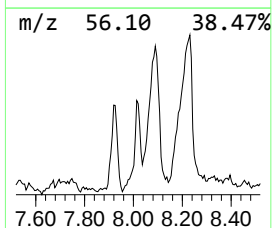
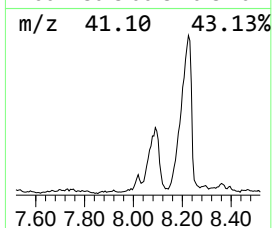
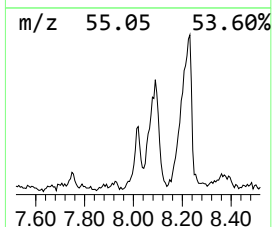
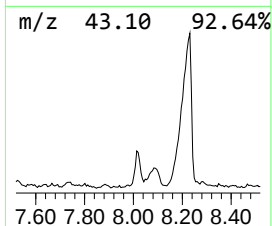
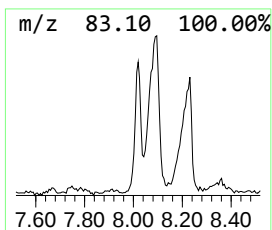
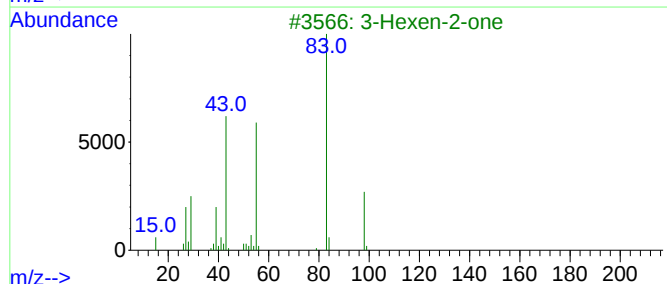
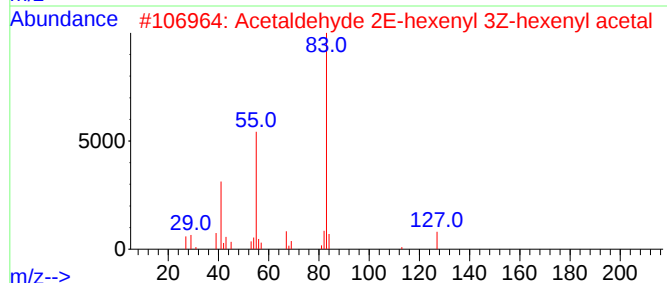
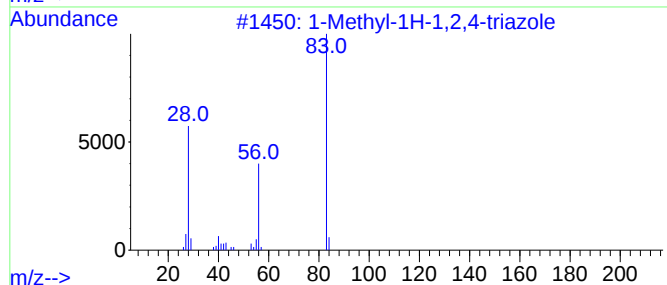
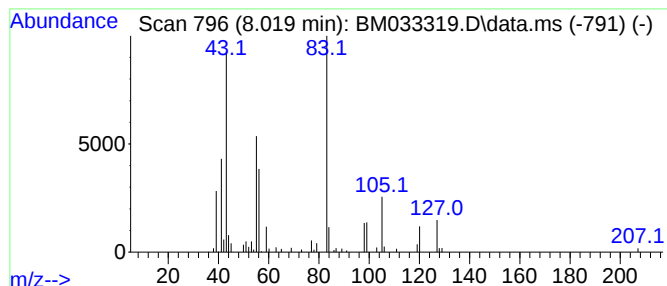
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown8.019 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.019	2.31 ng	87500	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	47
2			Acetaldehyde 2E-hexenyl 3Z-hexen...	226	C14H26O2	1000431-45-5	38
3			3-Hexen-2-one	98	C6H10O	000763-93-9	35
4			Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	32
5			1H-Azoline, octahydro-	127	C8H17N	005661-71-2	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
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Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
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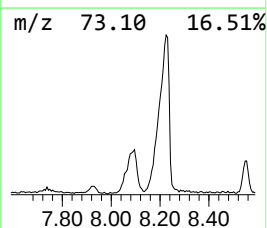
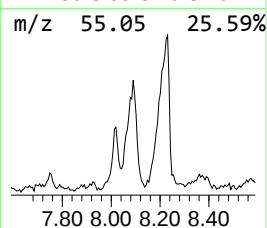
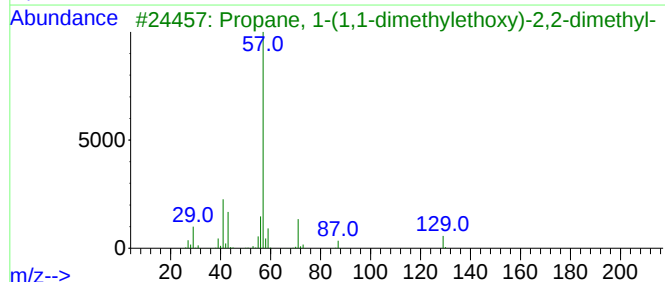
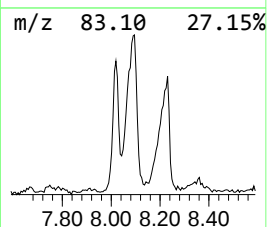
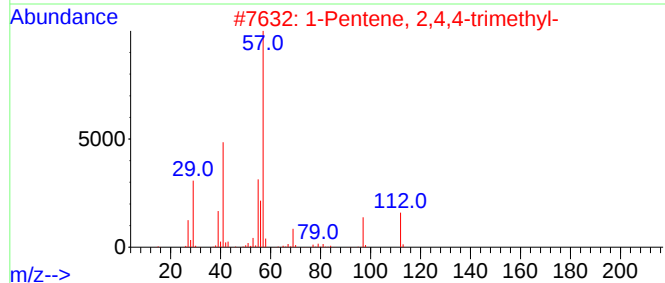
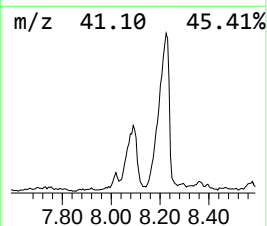
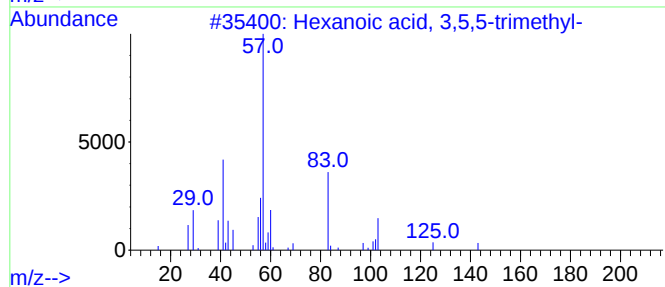
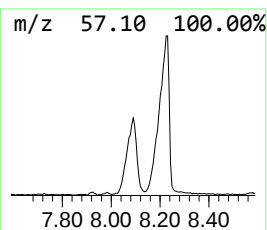
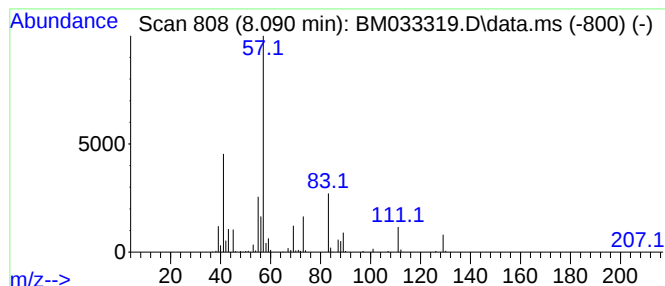
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown8.090 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.090	11.00 ng	415940	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	17
2			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	14
3			Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	14
4			2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	10
5			1-Propanol, 2,2-dimethyl-	88	C5H12O	000075-84-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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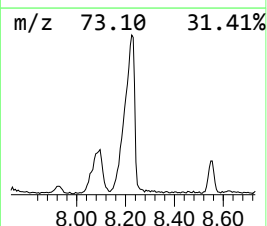
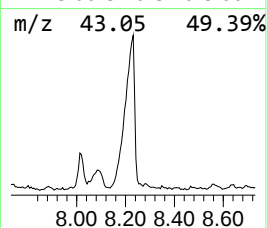
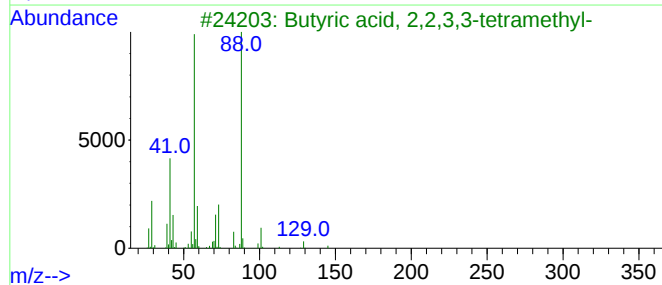
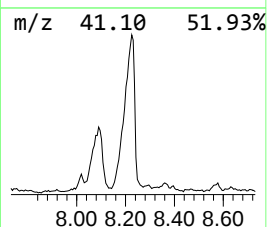
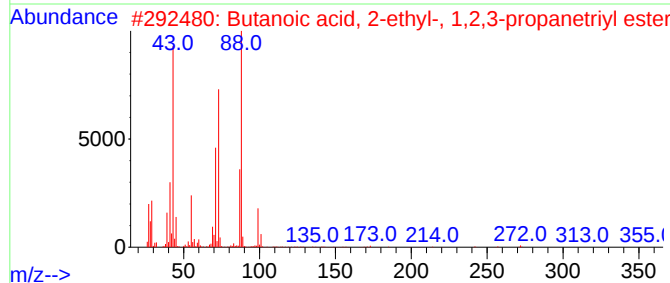
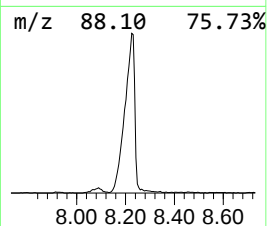
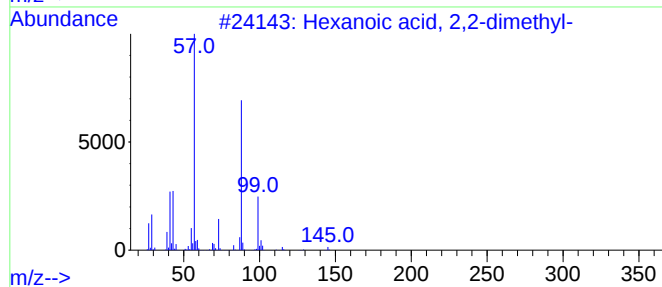
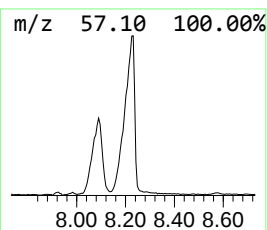
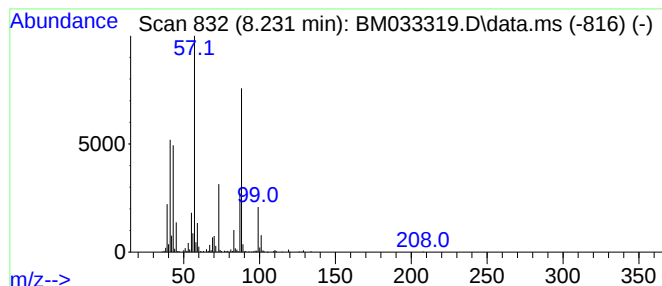
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Hexanoic acid, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.231	35.53 ng	1343810	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	59
2			Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	53
4			t-C4H9CH2C(O)OCH2CH3	144	C8H16O2	005340-78-3	40
5			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
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Misc :
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ClientSampleId :
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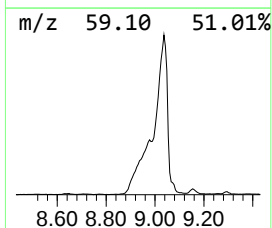
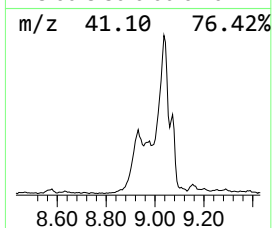
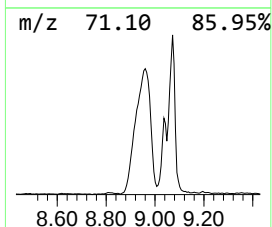
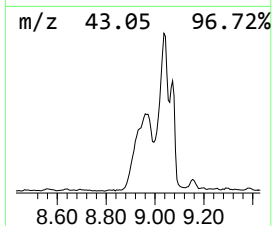
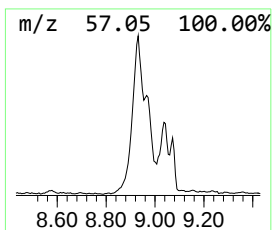
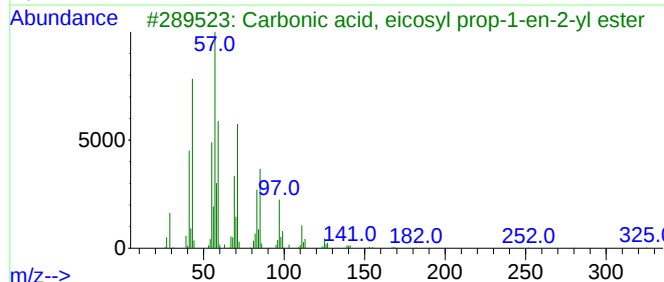
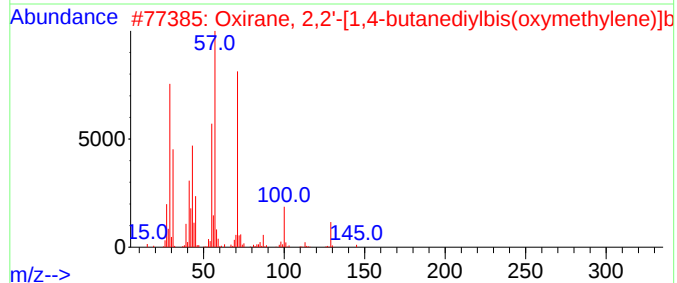
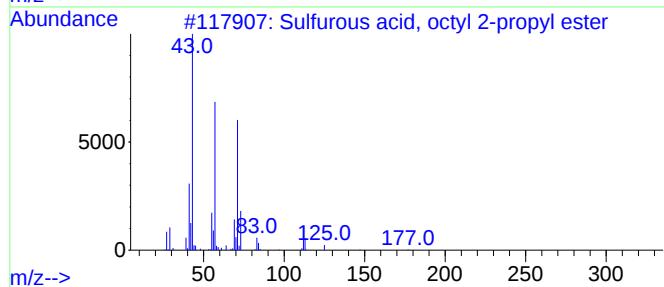
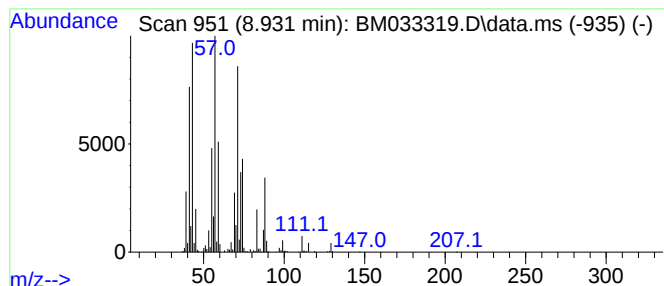
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown8.931 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.931	29.08 ng	1099970	1,4-Dichlorobenzene-d4	7.925

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, octyl 2-propyl e...	236	C11H24O3S	1000309-11-9	38
2			Oxirane, 2,2'-[1,4-butanediylbis...	202	C10H18O4	002425-79-8	38
3			Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	27
4			Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	27
5			Sulfurous acid, butyl pentyl ester	208	C9H20O3S	1000309-17-1	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
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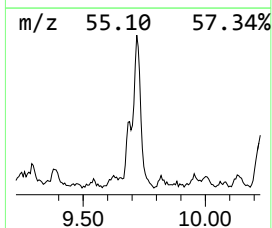
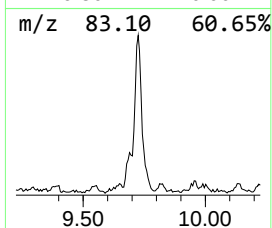
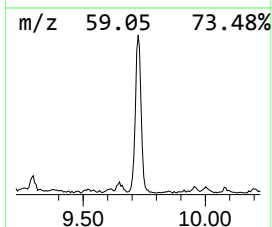
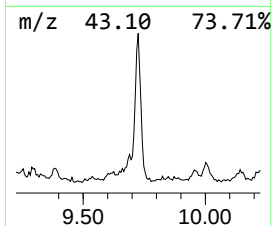
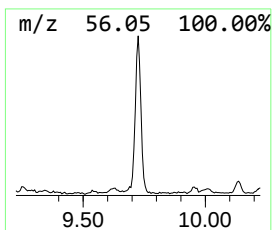
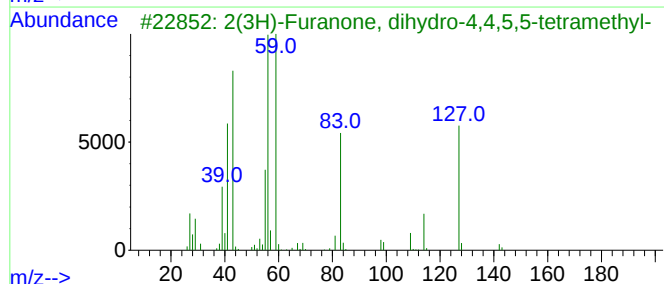
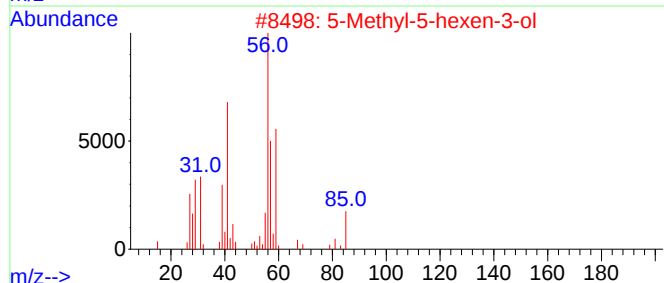
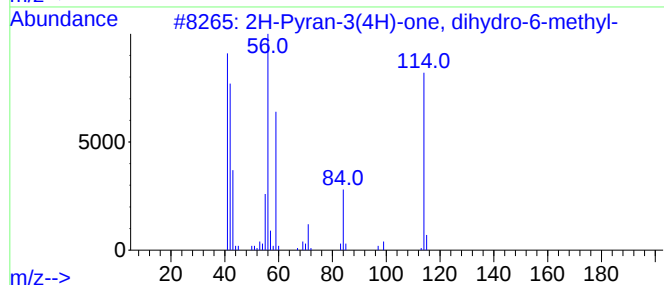
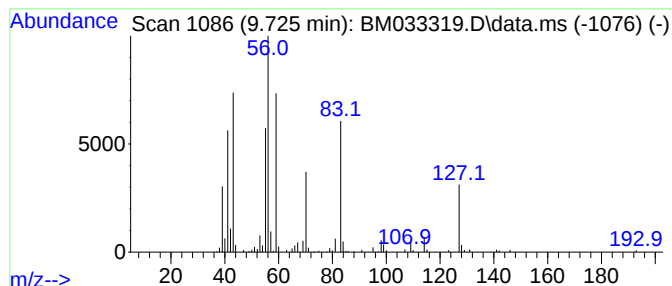
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2H-Pyran-3(4H)-one, dihydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.725	7.65 ng	424303	Naphthalene-d8	10.719

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2H-Pyran-3(4H)-one, dihydro-6-me...	114	C6H10O2	043152-89-2	50
2		5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	47
3		2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	43
4		Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	30
5		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
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Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

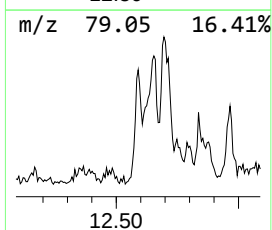
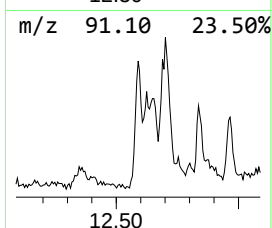
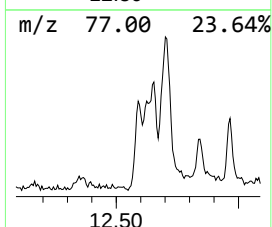
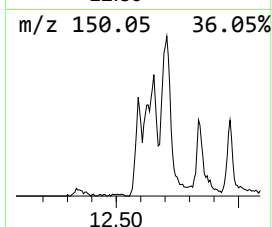
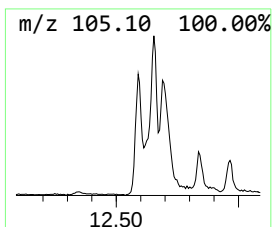
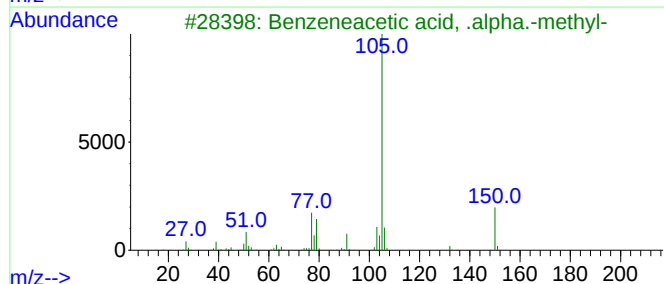
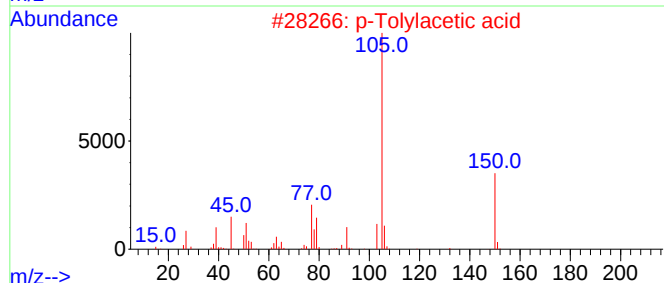
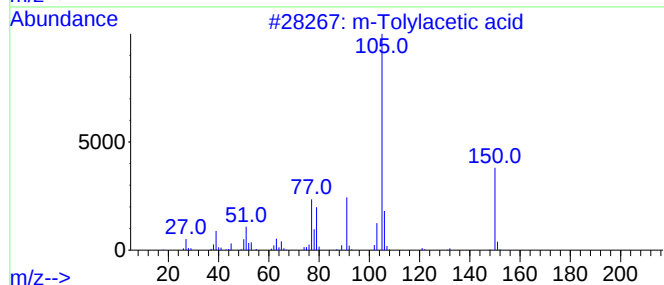
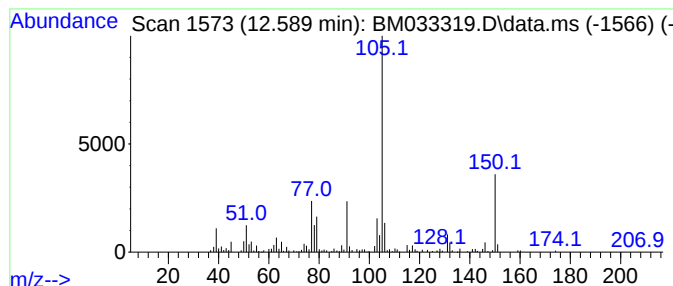
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BNA_M
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 m-Tolylacetic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.589	4.50 ng	249735	Naphthalene-d8	10.719	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	m-Tolylacetic acid	150	C9H10O2	000621-36-3	94
2	p-Tolylacetic acid	150	C9H10O2	000622-47-9	93
3	Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	90
4	Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	81
5	o-Tolylacetic acid	150	C9H10O2	000644-36-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-40

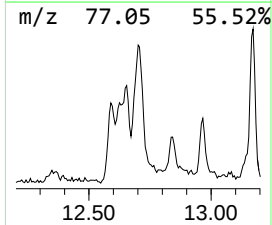
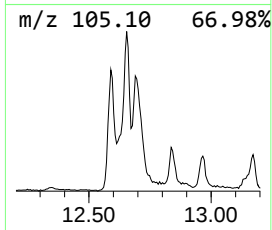
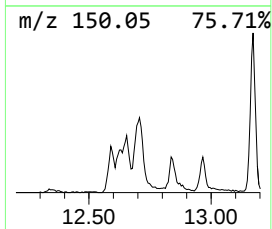
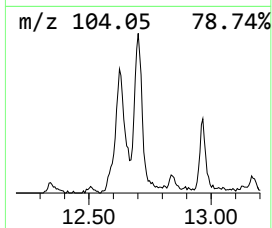
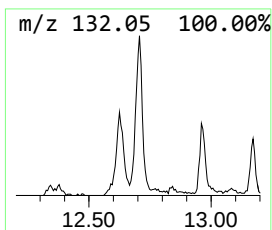
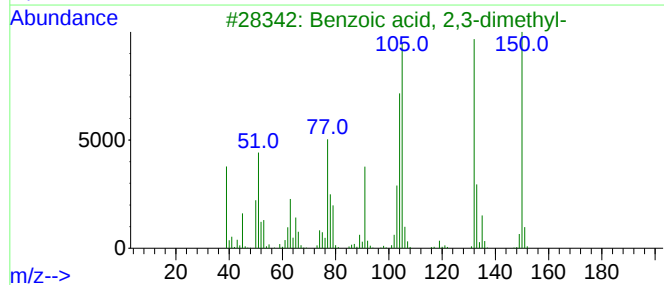
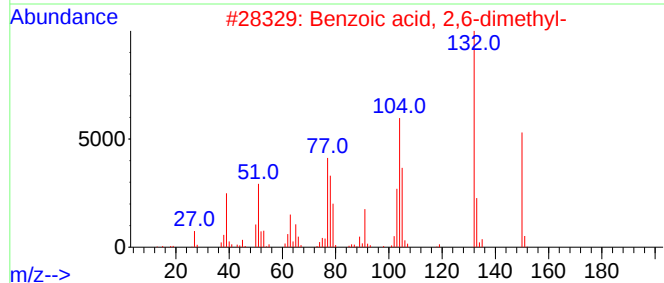
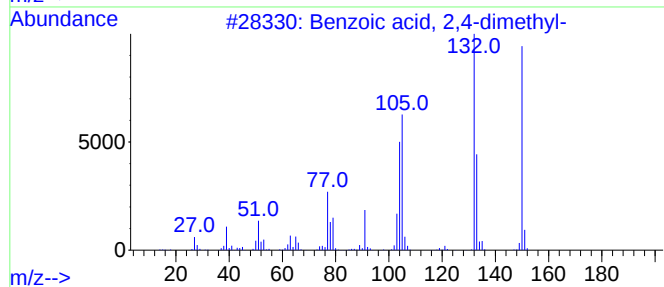
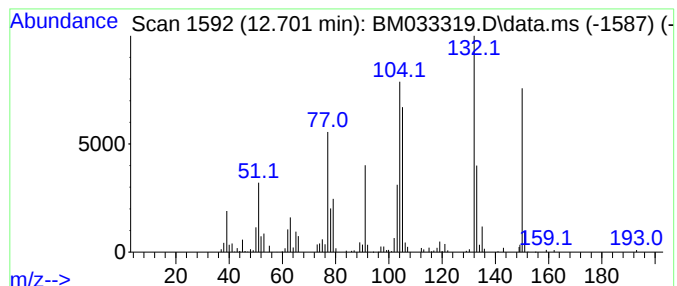
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Benzoic acid, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	6.06 ng	430750	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4-dimethyl-	150	C9H10O2	000611-01-8	87
2			Benzoic acid, 2,6-dimethyl-	150	C9H10O2	000632-46-2	83
3			Benzoic acid, 2,3-dimethyl-	150	C9H10O2	000603-79-2	76
4			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	58
5			Formic acid, 1-phenylethyl ester	150	C9H10O2	1000368-94-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-40

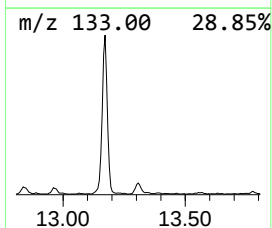
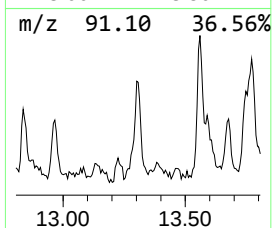
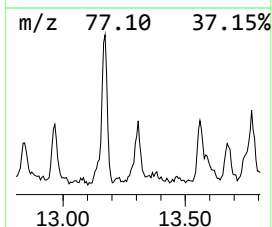
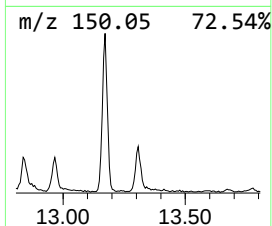
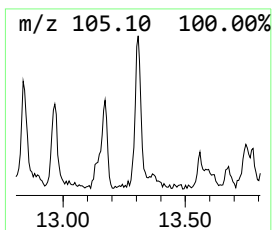
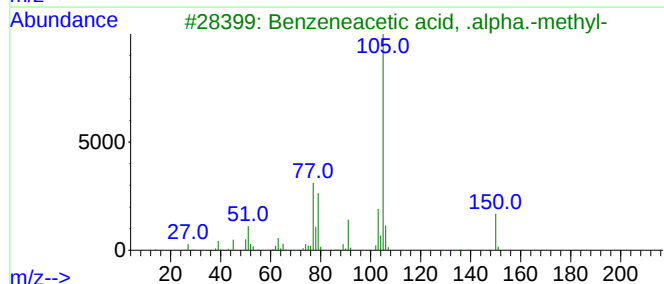
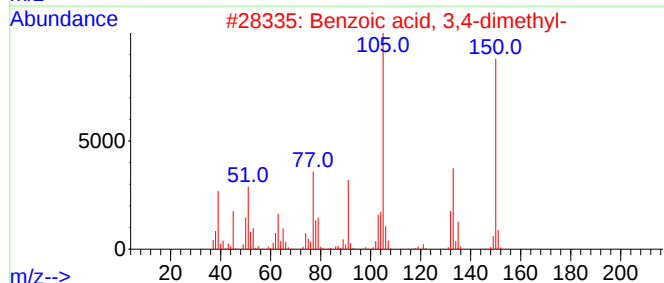
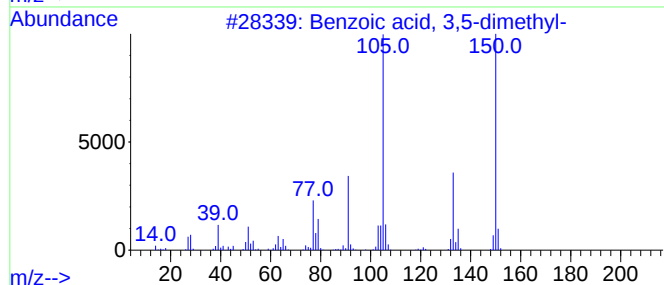
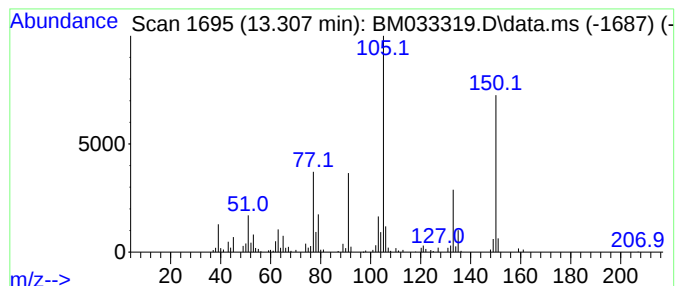
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Benzoic acid, 3,5-dimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.307	2.06 ng	146088	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3,5-dimethyl-	150	C9H10O2	000499-06-9	94
2			Benzoic acid, 3,4-dimethyl-	150	C9H10O2	000619-04-5	91
3			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	76
4			Benzoic acid, 2,5-dimethyl-	150	C9H10O2	000610-72-0	62
5			p-Tolylacetic acid	150	C9H10O2	000622-47-9	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-40

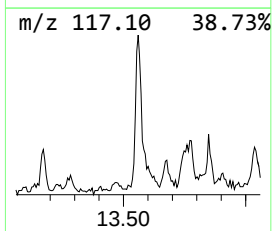
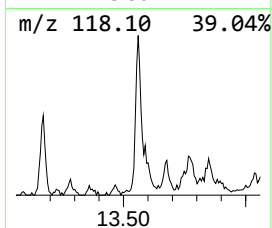
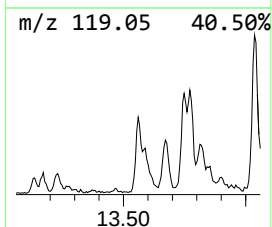
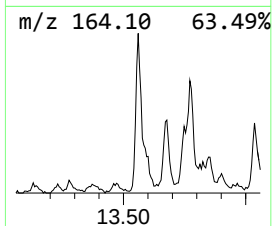
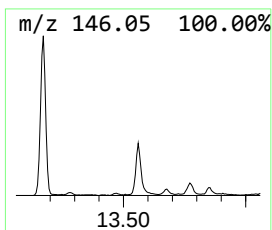
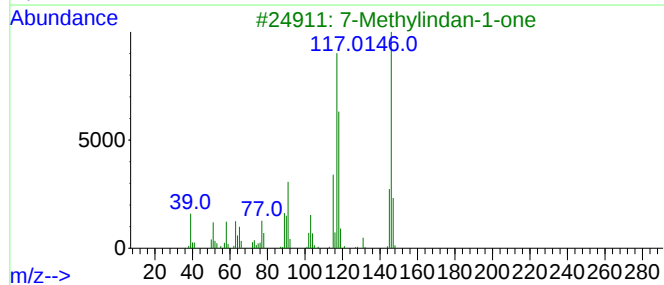
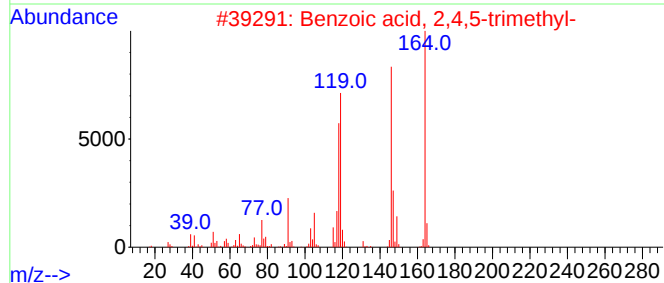
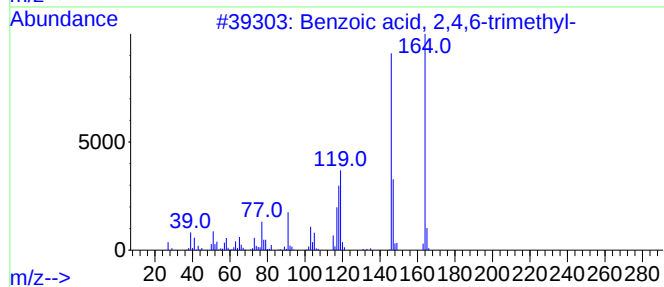
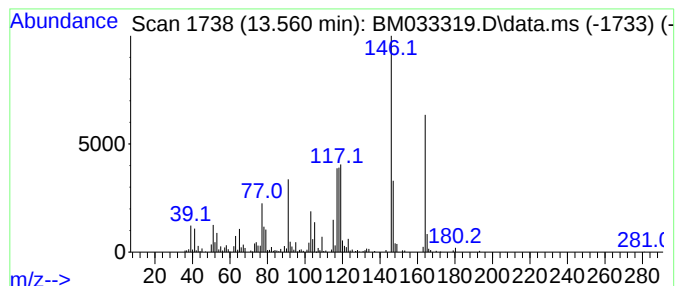
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzoic acid, 2,4,6-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.560	4.62 ng	328572	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	91
2			Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	50
3			7-Methylindan-1-one	146	C10H10O	039627-61-7	47
4			4-Pteridinecarboxylic acid, 7-me...	218	C10H10N4O2	016008-52-9	43
5			Cinnamaldehyde, .beta.-methyl-	146	C10H10O	001196-67-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-40

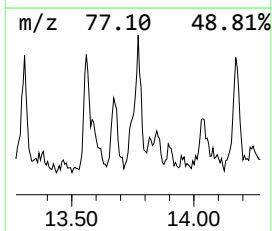
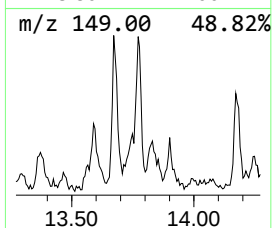
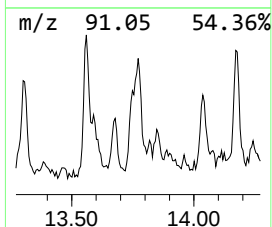
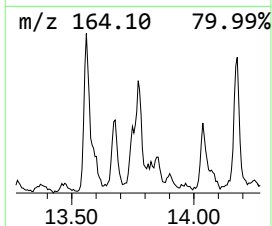
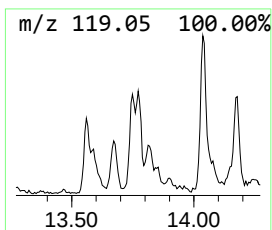
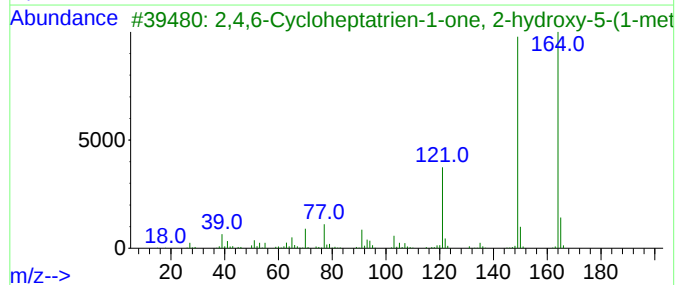
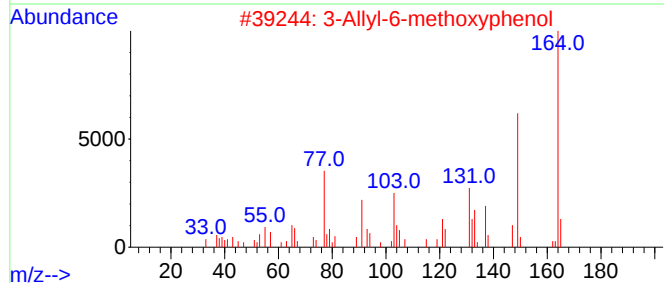
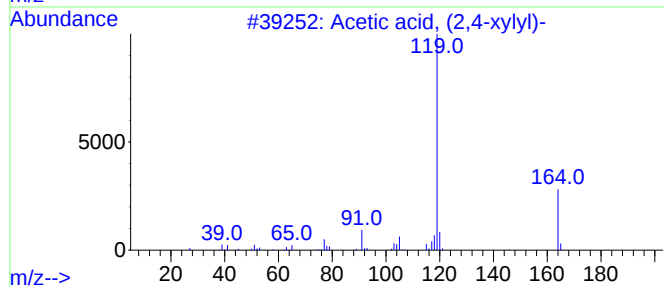
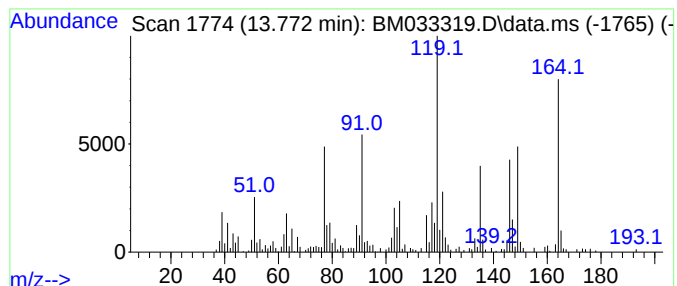
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Acetic acid, (2,4-xylyl)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.772	4.05 ng	288087	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	60
2			3-Allyl-6-methoxyphenol	164	C10H12O2	000501-19-9	38
3			2,4,6-Cycloheptatrien-1-one, 2-h...	164	C10H12O2	000672-76-4	38
4			Phenol, 2-methoxy-4-(1-propenyl)...	164	C10H12O2	005912-86-7	30
5			Phenol, 2-methoxy-4-(1-propenyl)-	164	C10H12O2	000097-54-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-40

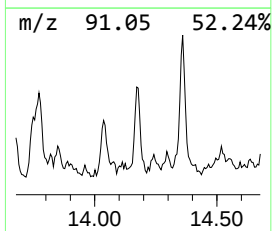
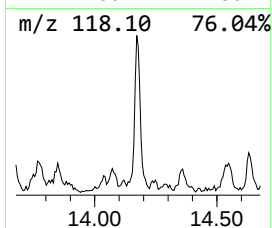
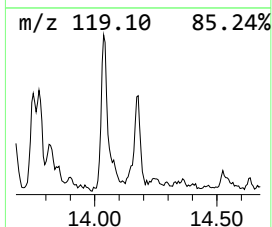
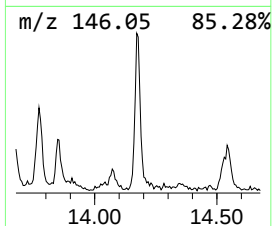
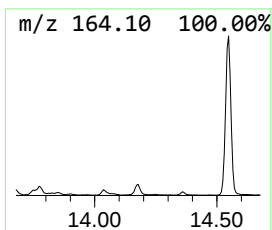
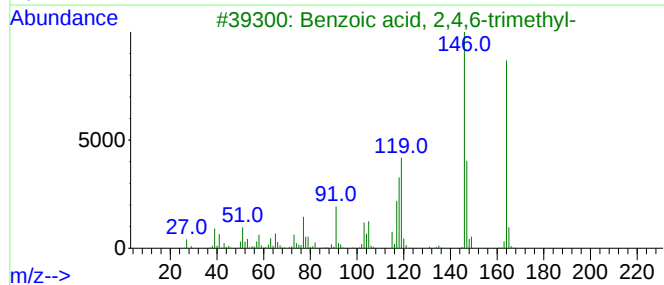
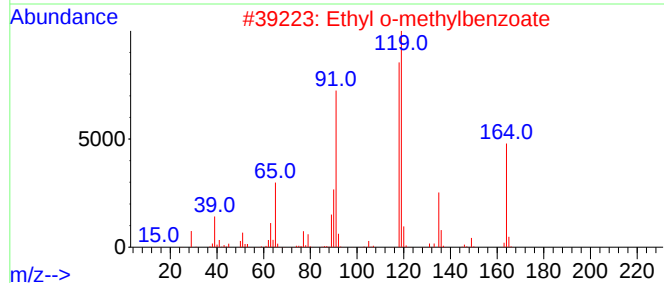
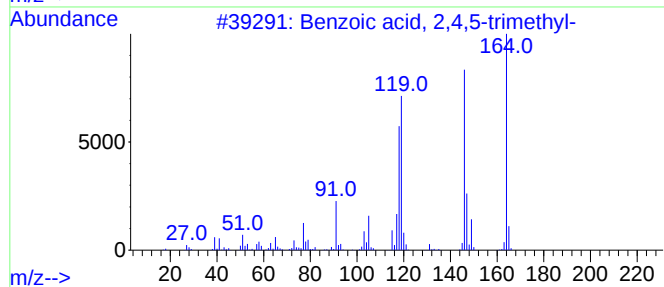
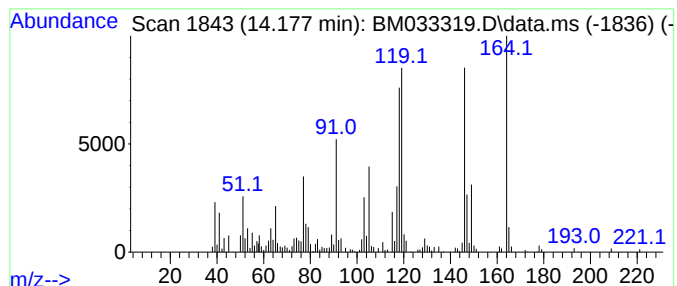
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Benzoic acid, 2,4,5-trimethyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.178	3.22 ng	229024	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2,4,5-trimethyl-	164	C10H12O2	000528-90-5	90
2			Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	60
3			Benzoic acid, 2,4,6-trimethyl-	164	C10H12O2	000480-63-7	46
4			2,5-Dimethylphenylacetic acid	164	C10H12O2	1000342-65-5	45
5			2-Propenoic acid, 3-(2-hydroxyph...	164	C9H8O3	000614-60-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
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Misc :
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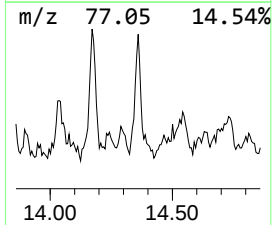
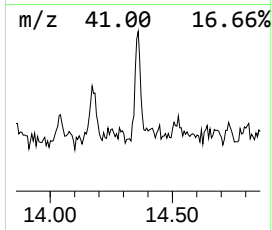
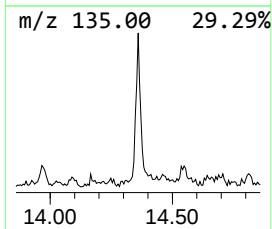
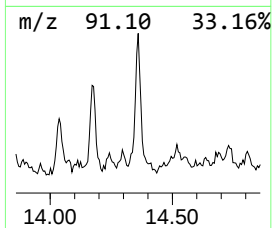
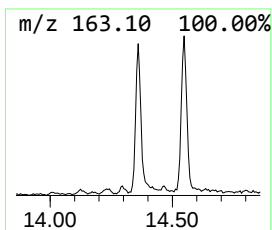
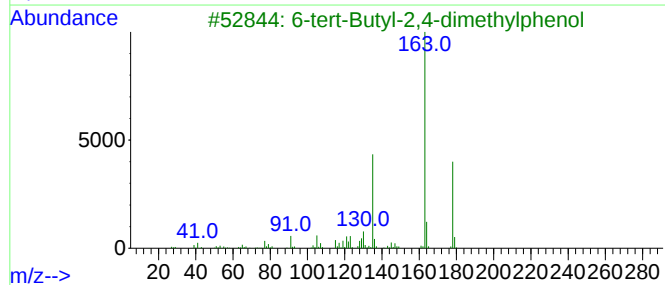
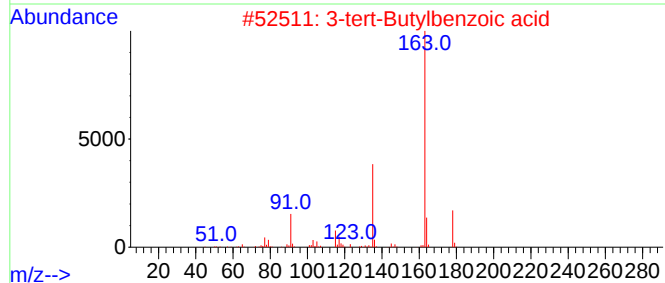
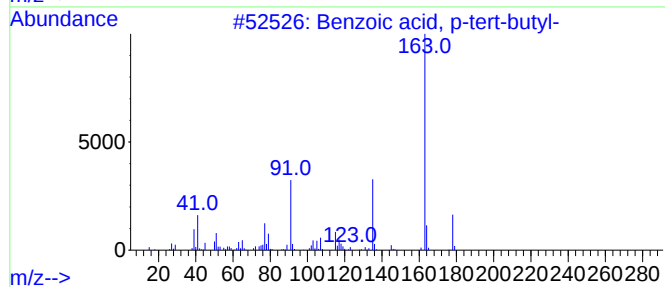
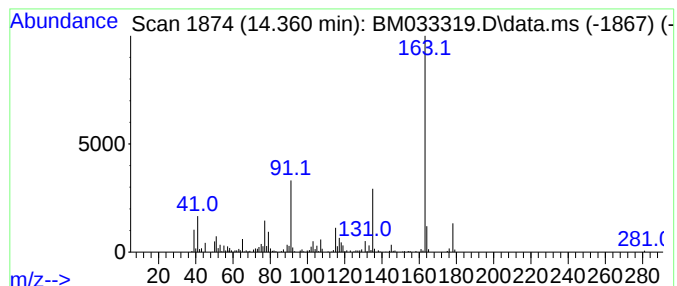
Instrument :
BNA_M
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Benzoic acid, p-tert-butyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.360	3.28 ng	232867	Acenaphthene-d10	14.548	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
2	3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	78
3	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
4	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	70
5	4-tert-Butyl-2,6-dimethylphenol	178	C12H18O	000879-97-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM120621\
Data File : BM033319.D
Acq On : 06 Dec 2021 19:12
Operator : CG/JU
Sample : M4918-06
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-40

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM112421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanol, 2,3-...	3.655	10.0	ng	377061	1	7.925	756494	20.0
1-Ethoxypentan-...	4.355	6.2	ng	234631	1	7.925	756494	20.0
Di-sec-Butyl ether	4.419	4.2	ng	157954	1	7.925	756494	20.0
3-Pentanone, 2,...	4.449	5.5	ng	208846	1	7.925	756494	20.0
unknown6.196	6.196	2.3	ng	87319	1	7.925	756494	20.0
Hydroxypivalic ...	7.343	5.0	ng	190063	1	7.925	756494	20.0
unknown8.019	8.019	2.3	ng	87500	1	7.925	756494	20.0
unknown8.090	8.090	11.0	ng	415940	1	7.925	756494	20.0
Hexanoic acid, ...	8.231	35.5	ng	1343810	1	7.925	756494	20.0
unknown8.931	8.931	29.1	ng	1099970	1	7.925	756494	20.0
2H-Pyran-3(4H)-...	9.725	7.7	ng	424303	2	10.719	1109370	20.0
m-Tolylacetic acid	12.589	4.5	ng	249735	2	10.719	1109370	20.0
Benzoic acid, 2...	12.701	6.1	ng	430750	3	14.548	1421460	20.0
Benzoic acid, 3...	13.307	2.1	ng	146088	3	14.548	1421460	20.0
Benzoic acid, 2...	13.560	4.6	ng	328572	3	14.548	1421460	20.0
Acetic acid, (2...	13.772	4.0	ng	288087	3	14.548	1421460	20.0
Benzoic acid, 2...	14.178	3.2	ng	229024	3	14.548	1421460	20.0
Benzoic acid, p...	14.360	3.3	ng	232867	3	14.548	1421460	20.0